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Fluid Dynamics Assessments of Deposition and Infiltration Models

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Fluid Dynamics Assessments of Deposition and Infiltration Models

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Abstract

The fluid dynamics assessments of deposition and infiltration models, such as the chemical-agent deposition analysis for rotorcraft surfaces (CADARS) and the aerosol and vapor infiltration analysis (AVIA) models, are carried out. Although these models address different needs of the Army and deal with enclosures surrounded by a toxic environment, we believe that there are enough similarities between them to be given the same type of fluid dynamics analysis.

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1. Introduction

Modeling of deposition and infiltration in general is, no doubt, a complex problem. Primarily, this is due to the fact that this modeling involves a great deal of fluid dynamics, which, however, cannot be solved exactly, forcing one to rely on approximate methods. An example of such a method is the Galerkin residual method, where one transforms the fluid equations from the differential forms into a matrix system of equations. Even with these kind of approximate methods, one still has a lot of work to do before satisfactory results are obtained. Sometimes, however, one may be able to avoid such difficult procedures by translating a difficult problem into a simpler one, which, however, still adequately represents the situation in practice. In fact, we show a specific example where this is the case when dealing with water droplets whose diameters are less than 5 mm; instead of droplets (which have only approximate shapes of spheres), these can actually be treated as rigid spheres with the same water density as droplets. Although our remarks will be of general nature, the emphasis in this report will be on two recent models (i.e., the chemical-agent deposition analysis for rotorcraft surfaces [CADARS] and aerosol and vapor infiltration analysis [AVIA] models).

Now, finding the appropriate approximate computational methods is just one of the problems. The other problem is the fact that helicopter cockpit (CADARS model) and the shelter with the communication gear (AVIA model) by themselves represent geometries of high complexities. Modeling how fluids behave inside and/or outside such complex geometries, even with approximate computational methods, is, generally, not a simple task.

In section 2, we give a general idea as to what CADARS and AVIA models are supposed to accomplish and, from the computational point of view, possible ways to do so. Section 3 deals with some specific physics type of questions for these models, while a discussion and a conclusion are given in section 4.

2. Descriptions of Models

The AVIA model is supposed to determine the infiltration of chemical-agent aerosols and vapors into an enclosure.

Initial development has been based on the S280 shelter, which is 5 ft × 5 ft × 7 ft. It can contain a lot of communication gear. The medium in a shelter is predominantly air; however, with one or more openings containing one or more obstacles and a pressure differential and/or concentration differential between the inside and the outside, one is faced with finding the amount and location of deposits and concentration of material in the interior of the shelter (i.e., in the air and on surfaces at any real time). On a specific level, to the model shelter (modeled after the S280 shelter), the average ballistic event is represented by about 37 holes. One hole has a 3-in diameter, and the rest of the 36 holes have a total surface area that is equivalent to the surface area of a single hole with the 3-in diameter. Clearly, the positions of the holes will affect the propagation of agents into the interior of the shelter. The most economical way to discuss the penetration of agents into the interior of the shelter is by employing the fluid dynamics, dynamically following the agent droplets through the holes, and seeing how and where they accumulate. This, of course, to be done properly, one needs the initial conditions of droplets before entering the shelter.

The CADARS computer model has been developed by Continuum Dynamics, Inc., under the contract with the U.S. Army Research Laboratory (ARL). It models the rotorcraft operating in a chemical-agent cloud by predicting the airflow around the airframe and using particle trajectory algorithms to determine the chemical-agent deposition on the airframe surface.

Essentially, the CADARS model is supposed to find out the mass deposition of harmful droplets on the helicopter panels; these panels are the result of subdividing the helicopter's surface into panels, about 7,340 in the case of the Comanche helicopter, in order to make the computations easier. Here, the problem is not just the deposition of droplets as the helicopter goes through a chemical cloud, but also the effects of rotor blades on this deposition. The chemical cloud is either

modeled as a constant concentration level or as the vapor, liquid, and solid tracking (VLSTRACK) computer model [1].

Regardless of whether we are dealing with the AVIA or the CADARS model, the problem, we believe, is essentially how to solve the fluid dynamics equations that incorporate inertial, as well as friction (viscous)-generated forces on the element of any portion of the fluid (gas). There is, however, a simple limit—the Knudsen gas limit—that one can take when dealing with the fluid/gas flow in a container (shelter or helicopter cockpit in this case). In this limit, no external (inertial or viscous) forces act on the fluid/gas molecules; the only forces are the ones from the interaction with the walls of the container. This is actually more realistic than it may sound. Namely, any rare gas, to a good approximation, is a Knudsen gas. Hence, when just taking a gas density to be small in flow simulations, one should obtain results that are consistent with a Knudsen gas; this, of course, will happen after a sufficiently long time when, in addition to gas density becoming low, the particle distribution becomes increasingly random.

Furthermore, as previously mentioned, the shelter or the cockpit of the helicopter represents a complex geometry. In order to simulate a fluid flow in such a geometry, one has to be very careful as to what method is used. Namely, even the finite-difference method, as opposed to the finite-element one, will yield very good and accurate results if the so-called Cartesian-structured meshes are employed; the advantage being that no explicit mesh-generation methods are needed and, therefore, greatly reduce human efforts involved in complex flow computations.

3. Some Physical Aspects of the Models

Let us first discuss the CADARS model. The mass deposition of harmful droplets will be affected not only by the speed of the helicopter, but also by the action of rotor blades as the helicopter goes through a chemical cloud. For the computational purposes, one actually calculates the mass deposition of harmful droplets on the helicopter panels; these panels, as mentioned earlier, are the result of subdividing the helicopter's surface. On average, there can be ~100 such flat panels;

the exact number depends on the desired accuracy of calculations. While the fluid dynamics methods that the contractor, Continuum Dynamics, uses appear to be adequate, the assumption that all of the droplets that hit the panels will actually stay there is a simplifying assumption that does not accurately represent the actual phenomenon.

We can try to remedy the situation by adding additional terms into the mass-rate accumulation equation that will make the droplet staying with the helicopter more realistic. For example, an additional term could even be an empirical term, which should be taken with the opposite sign and simply be proportional to the square of the helicopter velocity; as such, it would measure the "tearing" away of the droplets from the helicopter. This would happen faster with a larger velocity, and, with the suitable choice of the coefficient, it could be made negligible at small to normal velocities. Taking all of this into account, in fact, for the rate of droplet-mass deposition on the k-th panel, we can write the following equation:

$$\frac{dm}{dt} = -A_k \left(\hat{n}_k \cdot \vec{s}_k\right) \rho_d \left[1 - \frac{\left(\hat{n}_k \cdot \vec{s}_k\right)}{\left(\hat{n}_k \cdot \vec{s}_c\right)}\right], \qquad (1)$$

where A_k is the area of the k-th panel, ρ_d is the density of droplets, $\hat{n}_k$ the unit vector looking outwardly from the panel, $\vec{s}_k$ is the average droplet-fluid velocity at the k-th panel, and $\vec{s}_c$ is the critical average droplet-fluid velocity at which no more droplet-mass deposition occurs. Numerically, this velocity could be taken as velocity of sound.

Next, we discuss some physical aspects of the AVIA model. Taking into account that the model shelter will have 36 holes whose surface area equals that of a single 3-in hole, we see that on average, a diameter of the 36 holes is ~1 cm. As a consequence, it is safe to assume that droplets passing through these 36 holes will be less than 1 cm in diameter. Droplets of such small diameters undergo a minimum of deformations and can therefore be treated with the same type of equations of motion as for solid spheres with the droplet density. That, of course, simplifies the calculation

of droplet trajectories through air, which is described next for the special case of vertical motion by computing the vertical components of terminal velocities.

First of all, let us write down the equations of motion in the $x - y$ plane for a sphere (droplet) due to the viscous drag plus inertial (gravity plus buoyancy) forces. They are

$$(m + m')\frac{d^2x}{dt^2} = f_x, \tag{2a}$$

$$(m + m')\frac{d^2y}{dt^2} = f_y - (m - m_f)g, \tag{2b}$$

and

$$m' = \frac{m_f}{2}, \tag{2c}$$

where m_f is the mass of displaced fluid. Here we have chosen the y - axis to be the vertical axis parallel and antiparallel with buoyancy and gravitational forces, respectively. Next, we define various vector quantities with notation $\vec{V} = (V_x, V_y)$:

$$\vec{w} = (u, v) = \left(\frac{dx}{dt}, \frac{dy}{dt}\right) \tag{3}$$

is the velocity of the sphere situated at the position $\vec{r} = (x, y)$, while

$$\vec{w}_f = (u_f, v_f) \tag{4}$$

is the velocity of the fluid element at the position $\vec{r} = (x, y)$ in which the sphere is immersed. Finally, the relative velocity between the fluid element and the sphere at the position $\vec{r} = (x, y)$ is given as

$$\vec{w}_r = \vec{w}_f - \vec{w} = (u_f - u, v_f - v). \tag{5}$$

A very important case is when $\vec{w}_f = 0$; then

$$\vec{w}_f = 0 \rightarrow \vec{w}_r = -\vec{w}. \tag{6}$$

The viscous drag force $\vec{f}$ has the absolute value

$$f = |\vec{f}| = \frac{1}{8}\pi \rho_f d^2 c_d w_r^2, \tag{7a}$$

and

$$w_r = \sqrt{\vec{w}_r^2}, \ \vec{w}_r^2 = (u_f - u)^2 + (v_f - v)^2. \tag{7b}$$

Here, ρ_f is the fluid density, d is the diameter of the sphere, and c_d is the drag coefficient, which, in most cases, can be obtained from the Reynolds number R_e. In what follows, we shall assume it to be known for the velocities in question.

Now, if the sphere does not rotate, then $\vec{f} = (f_x, f_y)$ becomes a viscous drag in the direction of relative velocity $\vec{w}_r$. But this velocity makes an angle θ with x - axis; therefore, $\cos\theta = (u_f - u)/w_r$, and $\sin\theta = (v_f - v)/w_r$. This allows us to write the following expressions for the components of $\vec{f}$:

$$f_x = f\cos\theta = \frac{1}{8}\pi \rho_f c_d (u_f - u)\ w_r, \tag{8a}$$

and

$$f_y = f\sin\theta = \frac{1}{8}\pi \rho_f c_d (v_f - v)\ w_r. \tag{8b}$$

We are now ready to rewrite equations (2a), (2b), and (2c) in a true fluid dynamics form (i.e., without reference to masses explicitly). This is done by noticing that

$$m = \frac{4\pi d^3}{24}\rho, \tag{9a}$$

and

$$m_f = \frac{4\pi d^3}{24}\rho_f. \tag{9b}$$

When combining equations (2a), (2b), (2c), (7a), (7b), (8a), (8b), (9a) and (9b), we obtain

$$\frac{d^2x}{dt^2} = \frac{3\bar{\rho}}{4d\left(1 + \frac{\bar{\rho}}{2}\right)} c_d(u_f - u)w_r, \tag{10a}$$

$$\frac{d^2y}{dt^2} = \left(1 + \frac{\bar{\rho}}{2}\right)\left[-(1 - \bar{\rho})\, g + \frac{3\bar{\rho}}{4d} c_d\,(v_f - v)\, w_r\right], \tag{10b}$$

and

$$\bar{\rho} = \frac{\rho_f}{\rho}. \tag{10c}$$

These are a correct set of equations to determine positions of spheres. However, since they generally can be solved only numerically, they should be linearized, which facilitates their solutions through the so-called Runge-Kutta numerical methods. Their numerical solutions are beyond the scope of this report.

However, already from equation (10b), we can deduce that spheres (and or droplets) whose diameters are 5 mm or less should execute very similar dynamic motions, as long as their densities are the same. This, in fact, can be deduced analytically when the motion of the sphere is restricted to just a vertical direction.

To see this, we note that the left-hand sides of equations (10a) and (10b) are nothing more than accelerations in horizontal and vertical directions, respectively. Conveniently, they can be written in a vector form as $\vec{a} = (a_x, a_y)$. Next, let us simplify the situation by assuming that the fluid velocity satisfy $\vec{w}_f = 0$. Then, the relative velocity between the fluid element and the projectile (droplet) $\vec{w}_r$, at the position $\vec{r} = (x, y)$ is negative of the velocity of the sphere, $\vec{w}_r = -\vec{w}$. With these, our equations (10a) and (10b) now look like

$$\frac{d^2x}{dt^2} = -\frac{3\bar{\rho}}{4d\left(1 + \frac{\bar{\rho}}{2}\right)} c_d u w, \tag{11a}$$

$$\frac{d^2y}{dt^2} = \left(1 + \frac{\bar{\rho}}{2}\right)\left[-(1 - \bar{\rho})\, g - \frac{3\bar{\rho}}{4d}\, c_d v w\right], \tag{11b}$$

and

$$w = \sqrt{\vec{w}^{\,2}},\; \vec{w}^{\,2} = u^2 + v^2. \tag{11c}$$

It is easily seen that in the vertical direction, the sphere will reach a terminal velocity component, $v = -v_t$, where v_t now looks in a downward direction. This follows from the fact that acceleration in the vertical direction is zero, $a_y = 0$, when equation (11b) vanishes; that is, when

$$(1 - \bar{\rho})\, g - \frac{3\rho}{4d} c_d v_t \sqrt{u^2 + v_t^2} = 0. \tag{12}$$

We see that for every horizontal velocity component u there is a terminal vertical velocity component v_t.

Now we know that eventually in the horizontal direction, the sphere will stop moving, which we denote as the asymptotic case

$$u(\text{asymptotic}) = 0. \tag{13}$$

For the situation like this, or when u = 0 from the very beginning, from equation (12), we obtain the expression for the terminal vertical velocity component v_t to be

$$v_t = \sqrt{\frac{4g\,(1 - \bar{\rho})\, d}{c_d 3\bar{\rho}}}. \tag{14}$$

Of course if the initial conditions are such that the horizontal component of the sphere velocity is zero, then we would have only equation (11b) in the form

$$\frac{d^2y}{dt^2} = \left(1 + \frac{\bar{\rho}}{2}\right)\left[-(1 - \bar{\rho})\, g - \frac{3\bar{\rho}}{4d}\, c_d v|v|\right], \tag{15}$$

from which, when equated to zero, equation (14) follows immediately.

In order to compute v_t from equation (14), we have to specify some parameters. We wish to study the terminal velocities of "solid" water spheres of various diameters in air. Thus,

$$\rho = 1000.0 \text{ kg/m}^3, \ \rho_f = 1.22 \text{ kg/m}^3, \ \bar{\rho} = \frac{\rho_f}{\rho} = 0.0012, \text{ and } g = 9.8 \text{ m/s}^2. \tag{16}$$

Clearly, as equation (14) indicates, we also need to know c_d, the drag coefficient, which depends on the (dimensionless) Reynolds number R_e; generally, the dependence of C_d on R_e is only known empirically.

$$c_d = c_d\,(R_e), \tag{17}$$

where R_e, on the other hand, in terms of the sphere velocities [compare with equation (15)], is given as

$$R_e = \frac{wd}{\nu}, \tag{18a}$$

and

$$R_e(u = 0) = \frac{vd}{\nu}, \tag{18b}$$

where ν is the viscosity of the medium. For the air, its value is

$$\nu = 0.0000149 \text{ m}^2/\text{s}. \tag{19}$$

Implicitly, this makes c_d also dependent on w, or when u = 0, on v. Unfortunately, this dependence, again, is only empirical. Usually, in numerical computations, one takes R_e and, consequently, c_d from a last-step calculation assuming, of course, that it does not change too much as going from one step to the next (this one can verify afterwards).

In our case, this means that using equations (17), (18a), and (18b), we look for the converging result for v_t, as we start with some "arbitrary" initial $v_t \equiv v$. The process is as follows. Starting with initial v_t in equations (17), (18a), and (18b), we substitute the calculated c_d into equation (14), which yields a new v_t. This v_t is taken again as $v_t \equiv v$ in equations (17), (18a), and (18b), yielding a new c_d, which, in turn, is substituted into equation (14), giving an improved v_t. The process is repeated until the resulting v_t's do not change from each other. Of course, this procedure can be done only if the empirical equation (17) is known.

To be specific, we take

$$d = 0.001 \text{ m}. \tag{20}$$

Then, for step 0, we simply take for v_t the initial value,

$$\text{step (0):} \qquad v_t = 3 \text{ m/s}. \tag{21}$$

We use this for step (1).

$$\text{step (1):} \qquad R_e = 201.342. \tag{22}$$

For this kind of R_e's, the empirical equation (17) can be represented as [2]

$$c_d = \frac{24}{R_e^{0.646}}, \quad 1 < R_e \leq 400, \tag{23}$$

yielding for c_d:

$$\text{step (1):} \qquad c_d = 0.78. \tag{24a}$$

Combining these into equation (14) yields

step (1): $$v_t = 3.73408 \text{ m/s.} \tag{24b}$$

We now proceed with the step (2). From equation (18b) we have

step (2): $$R_e = 250.609, \tag{25a}$$

which, with the help of equation (23), gives

step (2): $$c_d = 0.68. \tag{25b}$$

Equation (14) gives

step (2): $$v_t = 3.999 \text{ m/s.} \tag{25c}$$

For step (3), we obtain

step (3): $$R_e = 268.389, \tag{26a}$$

$$c_d = 0.65, \tag{26b}$$

and

$$v_t = 4.1 \text{ m/s.} \tag{26c}$$

We take equation (26c) as a final value of v_t. The Reynolds number that goes with it is

$$R_e = 275.2 \tag{27}$$

According to Blanchard [2], the measured terminal velocity of the raindrop with $d = 0.001$ m is

$$v_t(\text{raindrop}) \cong 4 \text{ m/s,} \tag{28}$$

which indeed is very close to computed value of the terminal velocity of the solid water sphere, equation (26c).

One can do similar calculations for terminal velocities for other diameters for solid spheres of water and compare them with measured terminal velocities of rain droplets. The results are summarized in Table 1 [2]. From this table, one sees that the agreement between measured terminal velocities of a raindrop agrees very well with that computed for a rigid sphere for diameters less than 4.5 mm, or equivalently, for Reynolds numbers less than 3,000. Beyond these diameters and Reynolds numbers, while the terminal velocities keep increasing, the measured terminal velocities of raindrops are practically constant. Consequently, the calculations with rigid spheres will not approximate the real situation when $R_e \geq 3{,}000$. We believe that this is also true for other situations rather than just the terminal velocities.

Table 1. Comparison of Calculated Terminal Velocity of a Water—"Rigid Sphere" (With a Diameter d and calculated Reynolds number R_e) to Measured Terminal Velocity of a Raindrop

d (mm)	R_e	v_t (sphere) (m/s)	v_t (droplet) (m/s)
0.5	59	0.18	0.2
1.0	275	4.1	4.0
1.5	570	5.6	5.5
2.0	878	6.5	6.6
2.5	1227	7.4	7.5
3.0	1613	8.0	8.2
3.5	2033	8.7	8.7
4.0	2483	9.3	9.0
4.5	2963	9.8	9.1
5.0	3471	10.4	9.1
5.5	4004	10.8	9.2
6.0	4562	11.4	9.2

4. Discussion and Conclusion

The intent of the example with terminal velocities was to show that when using natural tricks, one may utilize fluid dynamics to address a variety of problems dealing with harmful liquids and vapors. While these problems may not be solved exactly according to the fundamental dynamic equations, nevertheless, these approximate methods may give completely satisfactory answers to practical problems that one is facing in the real world. The importance of terminal velocities themselves lies in the fact that droplets achieve them quickly as they travel through the air. Hence, one may obtain satisfactory answers to a variety of questions just by evaluating the terminal velocities. For example, the knowledge of terminal velocities should allow us to find the density of deposited chemical agent on objects inside the shelter after it entered. Furthermore, when a large size blob of fluid undergoes a breakup in the air, the resultant droplets will again achieve the respective terminal velocities quickly; these should then enable us to determine their distribution on the ground.

Therefore, when dealing with problems such as penetration and/or deposition of harmful chemical/biological compounds, the fluid dynamics, in a simple form, should, in the majority of cases, give completely satisfactory answers. We believe that equations (2a) through (11c) could be used as the basis for such a simplified treatment of deposition and infiltrations models of enclosed structures.

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The fluid dynamics assessments of deposition and infiltration models, such as the chemical-agent deposition analysis for rotorcraft surfaces (CADARS) and the aerosol and vapor infiltration analysis (AVIA) models, are carried out. Although these models address different needs of the Army and deal with enclosures surrounded by a toxic environment, we believe that there are enough similarities between them to be given the same type of fluid dynamics analysis.

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